

# The ground state of the carbon atom in strong magnetic fields

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(February 2, 2008)

The ground and a few excited states of the carbon atom in external uniform magnetic fields are calculated by means of our 2D mesh Hartree-Fock method for field strengths ranging from zero up to  $2.35 \cdot 10^9$  T. With increasing field strength the ground state undergoes six transitions involving seven different electronic configurations which belong to three groups with different spin projections  $S_z = -1, -2, -3$ . For weak fields the ground state configuration arises from the field-free  $1s^2 2s^2 2p_0 2p_{-1}$ ,  $S_z = -1$  configuration. With increasing field strength the ground state involves the four  $S_z = -2$  configurations  $1s^2 2s 2p_0 2p_{-1} 2p_{+1}$ ,  $1s^2 2s 2p_0 2p_{-1} 3d_{-2}$ ,  $1s^2 2p_0 2p_{-1} 3d_{-2} 4f_{-3}$  and  $1s^2 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$ , followed by the two fully spin polarized  $S_z = -3$  configurations  $1s 2p_0 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$  and  $1s 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 6h_{-5}$ . The last configuration forms the ground state of the carbon atom in the high field regime  $\gamma > 18.664$ . The above series of ground state configurations is extracted from the results of numerical calculations for more than twenty electronic configurations selected due to some general energetical arguments.

## I. INTRODUCTION

The behaviour and properties of atoms in strong magnetic fields is a subject of increasing interest. On the one hand this is motivated by the astrophysical discovery of strong fields on white dwarfs and neutron stars [1–3] and on the other hand the competition of the diamagnetic and Coulombic interaction causes a rich variety of complex properties which are of interest on their own. The carbon atom, which is the subject of the present investigation, plays a major role for the evolution of stars and is also expected to occur in the case of magnetic white dwarfs and neutron stars.

Investigations on the electronic structure in the presence of a magnetic field appear to be quite complicated due to the intricate geometry of this quantum problem. Most of the investigations in the literature focused on the hydrogen atom (for a list of references see, for example, [4–7]). The results of these studies provided us with an understanding of the absorption features of certain magnetic white dwarfs and allowed for a modeling of their atmospheres (see ref. [8] for a comprehensive review up to 1994 and ref. [9] for a more recent review on atoms and molecules in strong magnetic fields). On the other hand there is a number of magnetic white dwarfs whose spectra remain unexplained and cannot be interpreted in terms of magnetized atomic hydrogen. Furthermore new magnetic objects are discovered (see, for example, Reimers et al [10] in the course of the Hamburg ESO survey) whose spectra await to be explained. The most prominent of the unexplained magnetic objects is the white dwarf GD 229. Very recently significant progress has been achieved with respect to the interpretation of its rich spectrum ranging from the UV to the near IR. Extensive and precise calculations on the helium atom provided data for many excited states in a broad range of field strengths [11]. The comparison of the stationary transitions of the atom with the positions of the absorption edges of the observed spectrum yielded strong evidence for the existence

of helium in the atmosphere of GD229 [12].

For the hydrogen atom the impact of the competing Coulomb and diamagnetic interaction is particularly evident and pronounced in the intermediate regime for which the magnetic and Coulomb forces are comparable. For different electronic degrees of excitation of the atom the intermediate regime is met for different absolute values of the field strength. For the ground state this regime is roughly given by  $\gamma = 0.2 - 20$  ( $\gamma = B/B_0$  is the magnetic field strength in atomic units,  $B_0 = \hbar c/e a_0^2 = 2.3505 \cdot 10^5 \text{ T}$ ). Both early [13] and more recent works [4,14–17] on the hydrogen atom have used different approaches for relatively weak fields (the Coulomb force prevails over the magnetic force) and for very strong fields (the Coulomb force can be considered as weak in comparison with the magnetic forces which is the so-called adiabatic regime). In the latter regime the motion of the electron parallel to the magnetic field is dominated [18] by a 1D quasi-Coulomb potential including a parameter which depends on the magnetic field strength. The detailed calculations of the hydrogen energy levels carried out by Rösner *et al* [4] also retained the separation into different regimes of the field strength by decomposing the electronic wave function either in terms of spherical (weak to intermediate fields) or cylindrical (intermediate to high fields) orbitals. A powerful method to obtain comprehensive results on low-lying energy levels of the hydrogen atom in particular in the intermediate regime is provided by mesh methods [5].

For atoms with several electrons there are two decisive factors which enrich the possible changes in the electronic structure with varying field strength compared to the one-electron system. First we have a third competing interaction which is the electron-electron repulsion and second the different electrons feel very different Coulomb forces, i.e. possess different one particle energies, and consequently the regime of the intermediate field strengths appears to be the sum of the intermediate regimes for the separate electrons.

There exist a number of investigations on two-electron atoms in the literature [19–29]. The majority of them deals with the adiabatic regime in superstrong fields and the early works are mostly Hartree-Fock (HF) type calculations. There are also several early variational calculations for the low-field domain [21,30,31]. HF calculations for arbitrary field strengths have been carried out in refs. [4,26] by applying two different sets of basis functions in the high- and low-field regimes. As a result of the complicated geometry this approach suffers in the intermediate regime from very slow convergence and low accuracy of the calculated energy eigenvalues. Accurate HF calculations for arbitrary field strengths were carried out in refs. [25,27] by the 2D mesh HF method. Investigations on the ground state as well as a number of excited states of helium including the correlation energy have recently been performed via a Quantum Monte Carlo approach [29]. Very recently benchmark results with a precision of  $10^{-4} - 10^{-6}$  for the energy levels have been obtained for a large number of excited states with different symmetries using a configuration interaction approach with an anisotropic Gaussian basis set [11].

Focusing on systems with more than two electrons however the number of investigations is very scarce [23,28,32–34]. In view of the above there is a need for further quantum mechanical investigations and for data on atoms with more than two electrons in a strong magnetic field. For the carbon atom there exist only two investigations [23] in the adiabatic approximation which give a few values for the binding energies in the high field regime and one more relevant recent work by Jones *et al* [28]. The latter contains Hartree-Fock calculations for three states of the carbon atom in magnetic fields from  $\gamma = 0.0072$  up to  $\gamma = 21.6$ . The analysis of these results and in particular their comparison with our results are presented in sections IV and V.

In the current work we apply a fully numerical 2D Hartree-Fock method to the problem of the carbon atom in magnetic fields and obtain for the first time conclusive results on the ground state configurations

for arbitrary field strengths. Our approach enables us to perform calculations for various states with approximately equal precision for weak, intermediate and high magnetic fields. To identify the ground state for arbitrary field strengths both general considerations and electronic structure calculations have to be performed.

## II. COMPUTATIONAL METHOD

We solve the electronic Schrödinger equation for the carbon atom in a magnetic field under the assumption of an infinitely heavy nucleus in the (unrestricted) Hartree-Fock approximation. The numerical approach applied in the present work coincides with that of our previous investigations [33,34]. The latter contain some more details of the mesh techniques. The solution is established in the cylindrical coordinate system  $(\rho, \phi, z)$  with the  $z$ -axis oriented along the magnetic field. We prescribe to each electron a definite value of the magnetic quantum number  $m_\mu$ . Each one electron wave function  $\Psi_\mu$  depends on the variables  $\phi$  and  $(\rho, z)$  as follows

$$\Psi_\mu(\rho, \phi, z) = (2\pi)^{-1/2} e^{-im_\mu\phi} \psi_\mu(z, \rho) \quad (1)$$

where  $\mu$  indicates the numbering of the electrons. The resulting partial differential equations for  $\psi_\mu(z, \rho)$  and the formulae for the Coulomb and exchange potentials have been presented in ref. [27].

The one-particle equations for the wave functions  $\psi_\mu(z, \rho)$  are solved by means of the fully numerical mesh method described in refs. [5,27]. The feature which distinguishes the present calculations from those described in ref. [27] is the method of calculation of the Coulomb and exchange integrals. In the present work as well as in ref. [33,34] we obtain these potentials as solutions of the corresponding Poisson equation.

Our mesh approach is flexible enough to yield precise results for arbitrary field strengths. Some minor decrease of the precision appears in very strong magnetic fields. This phenomenon is due to a growing difference in the binding energies  $\epsilon_{B\mu}$  of one electron wave functions belonging to the same electronic configuration

$$\epsilon_{B\mu} = (m_\mu + |m_\mu| + 2s_{z\mu} + 1)\gamma/2 - \epsilon_\mu \quad (2)$$

where  $\epsilon_\mu$  is the one electron energy and  $s_{z\mu}$  is the spin  $z$ -projection. The precision of our results depends, of course, on the number of the mesh nodes and can be improved in calculations with denser meshes. Most of the present calculations are carried out on sequences of meshes with the maximal number of nodes being  $65 \times 65$ .

It was demonstrated in ref. [33] that the one electron wave functions obtained in multi-electron Hartree-Fock mesh calculations can for some atomic states possess a lower spatial symmetry than the symmetry constrained traditional HF approaches based on basis sets. For example it was shown [33] for the  $1s^2 2s^2$  state of the beryllium atom that the wave functions of the  $2s^2$  electrons reveal a broken spatial symmetry with respect to the  $z = 0$  plane. The contribution of this effect to the total energy was found to be significant for  $\gamma > 0.5$ . In the case of the carbon atom the  $2s^2$  electron pair belongs to the ground state configuration for the regime  $\gamma \leq 0.1862$  (see table I) for which the symmetry breaking effect does not occur. On the other hand, we do not expect such kind of a broken symmetry for the ground state configurations at strong magnetic fields because they involve wave functions with large absolute values of the magnetic quantum numbers. Due to these reasons the present calculations are based on one electron wave functions with a definite  $z$ -parity  $\pi_z = \pm 1$ .

### III. GROUND STATE ELECTRONIC CONFIGURATIONS FOR $\gamma = 0$ AND $\gamma \rightarrow \infty$

Let us provide some helpful qualitative considerations on the problem of the atomic multi-electron ground states in the limit of strong magnetic fields. It is clear that the field-free ground state of the carbon atom remains the ground state only for relatively weak fields. The set of one electron wave functions constituting the HF ground state for the opposite case of extremely strong magnetic fields can be determined as follows. The nuclear attraction energies and HF potentials (which determine the motion along  $z$  axis) are for large  $\gamma$  small compared to the interaction energies with the magnetic field (which determines the motion perpendicular to the magnetic field and is responsible for the Landau zonal structure of the spectrum). Thus, all the one electron wave functions must correspond to the lowest Landau zones, i.e.  $m_\mu \leq 0$  for all the electrons, and the system must be fully spin-polarized, i.e.  $s_{z\mu} = -\frac{1}{2}$ . For the Coulomb central field the one electron levels form quasi 1D Coulomb series with the binding energy  $E_B = \frac{1}{2n_z^2}$  for  $n_z > 0$  and  $E_B \rightarrow \infty$  for  $n_z = 0$ , where  $n_z$  is the number of nodal surfaces of the wave function crossing the  $z$  axis.

Considering the case  $\gamma \rightarrow \infty$  it is evident, that the wave functions with  $n_z = 0$  have to be chosen for the ground state configuration. Furthermore starting with the energetically lowest one particle level the electrons occupy according to the above arguments orbitals with increasing absolute value of the magnetic quantum number  $m_\mu$ . Consequently the ground state of the carbon atom must be given by the configuration  $1s2p_{-1}3d_{-2}4f_{-3}5g_{-4}6h_{-5}$ .

For the opposite case  $\gamma = 0$  it is well-known that the ground state of the carbon atom corresponds to the spectroscopic term  $^3P$ . In the framework of the non-relativistic consideration this term consists of nine states degenerate due to three possible  $z$ -projections of the total spin  $S_z = -1, 0, 1$  and three possible values of the total magnetic quantum number  $M = -1, 0, 1$ . Conventional Hartree-Fock calculations provide the following values for the energy for this term:  $E = -37.688612$  (Clementi and Roetti in [35]) and  $E = -37.68880$  (Froese Fischer in [36]).

The problem of the configurations of the ground state for the intermediate field region cannot be solved without doing explicit calculations combined with some qualitative considerations in order to extract the relevant configurations. With respect to our notation of the configurations we implicitly assume in the following that all paired electrons, like for example the  $1s^2$  part of a configuration, are of course in a spin up and spin down orbital, respectively, whereas all unpaired electrons possess a negative projection of the spin onto the magnetic field direction.

### IV. GROUND STATE ELECTRONIC CONFIGURATIONS FOR ARBITRARY FIELD STRENGTHS

First of all, we divide the possible ground state configurations into three groups according to their total spin projection  $S_z$ : the  $S_z = -1$  group (low-field ground state configurations), the intermediate group  $S_z = -2$  and the  $S_z = -3$  group (the high-field ground state configurations). This grouping is required for the following qualitative considerations which are based on the geometry of the spatial parts of the one electron wave functions.

To begin we would like to remark on our calculations for the atom without field compared to the traditional Hartree-Fock calculations. The Hartree-Fock energies for the  $^3P$  ground state of the field-free carbon atom have been given above. One important feature of the conventional Hartree-Fock calculations

[35,36] is the correspondence of each one electron wave function to only one spherical harmonic. As shown for example in ref. [33] this restriction does not allow obtaining energies which correspond to the Hartree-Fock limit in the sense of a fully free variation of the one-particle functions respecting the exact symmetries of the total system. Not imposing the symmetries of the spherical harmonics on the one-particle functions provides lower Hartree-Fock energies. This can be done, for instance, in 2D or 3D mesh Hartree-Fock calculations. In the framework of our 2D mesh calculations the components of the multiplet  $^3P$  are built up of different one particle wave functions possessing as good quantum numbers the magnetic quantum number  $m_l$ , the  $z$ -parity and the spin projection  $s_z$ . Due to the higher flexibility of the one particle wave functions our Hartree-Fock energies for all the components of the  $^3P$  multiplet are lower in energy and are slightly different for different components of the multiplet. At  $\gamma = 0$  the value of  $S_z$  does not affect the energy, whereas the spatial parts can contain three valence configurations:  $2p_0 2p_{-1}$ ,  $2p_0 2p_{+1}$  and  $2p_{-1} 2p_{+1}$  (the core part  $1s^2 2s^2$  of the total configuration is omitted). Our energies for the  $2p_0 2p_{-1}$  and  $2p_0 2p_{+1}$  configurations coincide and are  $E = -37.69096$ , whereas the calculation for  $2p_{-1} 2p_{+1}$  gives a slightly different value namely  $E = -37.69376$ . It is evident that the energies of these configurations must coincide in 3D HF calculations. On the other hand only the  $1s^2 2s^2 2p_0 2p_{-1}$  configuration represents the energetically lowest component of the  $^3P$  multiplet in weak magnetic fields. We therefore neglect here and in the following the small difference in energy of the  $1s^2 2s^2 2p_0 2p_{+1}$ ,  $1s^2 2s^2 2p_{-1} 2p_{+1}$   $1s^2 2s^2 2p_0 2p_{-1}$  configurations in the absence of a magnetic field.

According to the arguments presented in the previous section we know that the ground state configuration of the carbon atom in the high field limit must be the fully spin-polarized state  $1s 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 6h_{-5}$ . The question of the ground state configurations at intermediate fields cannot be solved without performing explicit electronic structure calculations. On the other hand, the a priori set of possible intermediate ground state configurations increases enormously with increasing number of electrons and is already for the carbon atom too many in order to perform explicit calculations for all of them. Some qualitative considerations are therefore needed in order to exclude certain configurations as possible ground state configurations thereby reducing the number of candidates for which explicit calculations have to be performed. The optimal strategy hereby consists of the repeated procedure of determining neighbouring ground state configurations with increasing (or decreasing) magnetic field strength using both qualitative arguments (see below) as well as the results of the calculations for concrete configurations.

The energies for all the considered states and in particular those of the ground states are illustrated in figures 1-4. Figure 1 shows the total energies for the considered configurations with  $S_z = -1$ . Figure 2 and 3 illustrate the intermediate ground state scenario for the relevant configurations possessing the spin projection  $S_z = -2$ . Figure 4 shows the relevant fully spin polarized configurations, i.e. the states with  $S_z = -3$ . The reader should note that for each group of configurations the figures illustrate a different regime of field strengths and energies. Finally we present in figure 5 the global scenario of the total energies of the ground states for the range of considered field strength  $0 < \gamma < 100 a.u.$  The vertical lines shown in this picture divide the complete field strength regime into different regions for which different electronic configurations represent the ground state. The numerical values for the transition field strengths and the total energies at which the crossover between different electronic configurations takes place are given in table I. In the following paragraphs we describe in detail our selection procedure for the candidates of the electronic ground state configurations.

We start our consideration for  $\gamma \neq 0$  with the high-field ground state and subsequently consider other possible candidates in question for the electronic ground state for  $S_z = -3$  (see figure 4) *with decreasing*

*field strength.* All the one electron wave functions of the high-field ground state  $1s2p_{-1}3d_{-2}4f_{-3}5g_{-4}6h_{-5}$  possess no nodal surfaces crossing the  $z$ -axis and occupy the energetically lowest orbitals with magnetic quantum numbers ranging from  $m = 0$  down to  $m = -5$ . We shall refer to the number of the nodal surfaces crossing the  $z$  axis as  $n_z$ . The  $6h_{-5}$  orbital possesses the smallest binding energy of all orbitals constituting the high-field ground state. Its binding energy decreases rapidly with decreasing field strength. Thus, we can expect that the first crossover of ground state configurations happens due to a change of the  $6h_{-5}$  orbital into one possessing a higher binding energy at the corresponding lowered range of field strength. It is natural to suppose that the first transition while decreasing the magnetic field strength will involve a transition from an orbital possessing  $n_z = 0$  to one for  $n_z = 1$ . The energetically lowest available one particle state with  $n_z = 1$  is the  $2p_0$  orbital. Another possible orbital into which the  $6h_{-5}$  wave function could evolve is the  $2s$  state. For the hydrogen atom or hydrogen-like ions in a magnetic field the  $2p_0$  is stronger bound than the  $2s$  orbital. On the other hand, owing to the electron screening in multielectron atoms in field-free space the  $2s$  orbital tends to be more tightly bound than the  $2p_0$  orbital. Thus, two states i.e. the  $1s2p_02p_{-1}3d_{-2}4f_{-3}5g_{-4}$  state as well as the  $1s2s2p_{-1}3d_{-2}4f_{-3}5g_{-4}$  configuration are candidates for becoming the ground state in the  $S_z = -3$  set when we lower the field strength coming from the high field situation.

Analogous arguments lead to the three following candidates for the ground state in case of the second crossover in the  $S_z = -3$  subset which takes place with decreasing field strength:  $1s2s2p_02p_{-1}3d_{-2}4f_{-3}$ ,  $1s2p_02p_{-1}3d_{-1}3d_{-2}4f_{-3}$  and  $1s2s2p_{-1}3d_{-1}3d_{-2}4f_{-3}$ . It is evident that the one particle energies for the  $3d_{-1}$  and  $2p_0$  obey  $E_{3d_{-1}} > E_{2p_0}$  for all values of  $\gamma$  since they possess the same nodal structure with respect to the  $z$ -axis and only the  $3d_{-1}$  possesses an additional node in the plane perpendicular to the  $z$ -axis. For this reason the configuration  $1s2s2p_{-1}3d_{-1}3d_{-2}4f_{-3}$  can be excluded from our considerations of the ground state. This conclusion is fully confirmed by our calculations.

The final picture of the ground state crossovers in the subset of configurations with  $S_z = -3$  obtained within our HF calculations is the following: At  $\gamma \approx 18.664$  the total energy  $E(\gamma)$  for the  $1s2p_02p_{-1}3d_{-2}4f_{-3}5g_{-4}$  configuration intersects the total energy curve for the high-field ground state  $1s2p_{-1}3d_{-2}4f_{-3}5g_{-4}6h_{-5}$  and for  $\gamma < 18.664$  the energy of the previous state is therefore lower than the energy of the high-field ground state. The  $1s2p_02p_{-1}3d_{-2}4f_{-3}5g_{-4}$  configuration remains the energetically lowest one among all the six above-considered states with  $S_z = -3$  in the regime  $6.8 < \gamma < 18.664$ . For  $\gamma < 6.8$  the configuration  $1s2s2p_02p_{-1}3d_{-2}4f_{-3}$  becomes the lowest one within the  $S_z = -3$  subset. However, this second crossover within the subset of states with  $S_z = -3$  takes place in a regime of field strengths for which the global ground state configuration of the carbon atom belongs already to the subset  $S_z = -2$ . (See the state  $1s^22p_{-1}3d_{-2}4f_{-3}5g_{-4}$  in figure 4.) It should be noted that the structure of the wave functions with  $S_z = -3$  is simpler than in the two other spin subsets which we consider in the following.

The considerations for the  $S_z = -2$  subset of states whose energies are illustrated in figures 2 and 3, are similar to the ones of the subset  $S_z = -3$ . The most tightly bound state in the limit of high fields is given by the  $1s^22p_{-1}3d_{-2}4f_{-3}5g_{-4}$  configuration. When decreasing the field strength this configuration can be replaced by  $1s^22p_02p_{-1}3d_{-2}4f_{-3}$  or by  $1s^22s2p_{-1}3d_{-2}4f_{-3}$  (see figure 3). The next change could lead to the configurations  $1s^22s2p_02p_{-1}3d_{-2}$ ,  $1s^22p_02p_{-1}3d_{-1}3d_{-2}$  or  $1s^22s2p_{-1}3d_{-1}3d_{-2}$  (figure 3). In analogy to our argumentation with the subset of states with  $S_z = -3$  it is now obvious that  $E_{1s^22s2p_02p_{-1}3d_{-2}} < E_{1s^22s2p_{-1}3d_{-1}3d_{-2}}$  and the latter state cannot become the ground state configuration. Our electronic structure calculations provide the following sequence of ground states for decreasing field strength: for high fields we have the  $1s^22p_{-1}3d_{-2}4f_{-3}5g_{-4}$  configuration, with decreas-

ing field strength a crossover to the configuration  $1s^2 2p_0 2p_{-1} 3d_{-2} 4f_{-3}$  and with further decreasing field strength the configuration  $1s^2 2s 2p_0 2p_{-1} 3d_{-2}$ . Having in mind these numerical results which are presented in figure 3 we provide next an analysis for further decreasing field strength. It is clear that the orbitals  $1s^2$  and  $2s 2p_0 2p_{-1}$  will be retained for further decreasing field strength in the framework of the  $S_z = -2$  subspace. Thus the following transitions can affect only the orbital  $3d_{-2}$ . This orbital could be changed to the orbitals  $3d_{-1}$ ,  $3d_0$ ,  $3p_{-1}$ ,  $3s$  or  $2p_{+1}$ . The  $d$ -orbitals of this series can be excluded from our consideration, since they have no preferences over  $3d_{-2}$  with respect to the energy neither in strong nor in weak fields and therefore calculations have to be performed only for the states  $1s^2 2s 2p_0 2p_{-1} 3p_{-1}$ ,  $1s^2 2s 2p_0 2p_{-1} 3s$  and  $1s^2 2s 2p_0 2p_{-1} 2p_{+1}$ . Explicit calculations (see figure 2) show that the ground state is given by the  $1s^2 2s 2p_0 2p_{-1} 2p_{+1}$  configuration. It is evident that the latter configuration is the ground state configuration of the subset  $S_z = -2$  for the weak field regime and in particular for  $\gamma = 0$  and thus it is the last in the sequence of the ground state configurations with  $S_z = -2$ . As it turns out in our HF calculations this state as well as all other states which are ground states for  $S_z = -2$  turn out to be the ground state of the carbon atom as a whole, i.e. taking into account all spin manifolds  $S_z$ , for certain regimes of the field strength.

It is reasonable to start the considerations for the configurations with  $S_z = -1$  which includes the weak field ground state configuration  $1s^2 2s^2 2p_0 2p_{-1}$  by gradually increasing the field strength from  $\gamma = 0$ . The configuration  $1s^2 2s^2 2p_0 2p_{-1}$  is rather robust and the most reasonable transition which could occur in the framework of the configurations with  $S_z = -1$  is the transition of one of the  $2s$  electrons to the  $2p_{-1}$  orbital i.e. the transition to configuration  $1s^2 2s 2p_0 2p_{-1}^2$ . The argument therefore is that at  $\gamma = 0$  the  $2s$  orbital is more bound than the  $2p_0$  and  $2p_{-1}$  and for increasing the field the binding energy of the  $2p_{-1}$  orbital increases very rapidly. Our explicit calculations (see figure 1) show that this transition takes place at  $\gamma \approx 0.7$ , i.e. in the regime, for which the ground state configuration belongs already to the subset  $S_z = -2$ . In addition to several other configurations with  $S_z = -1$  we have also performed calculations for the configuration  $1s^2 2s^2 2p_{-1}^2$  belonging to  $S_z = 0$ , which is also presented in figure 1. This configuration with the symmetry  $^1D$  is the ground state of the subset  $S_z = 0$  at  $\gamma = 0$ . The calculations for this state were necessary in order to exclude the possibility that it becomes the ground state of the carbon atom for some region of the field strength in the weak field case.

The results of the investigations of this section are presented in table I which contains the critical values of  $\gamma$  at which the crossovers of different ground state configurations take place (see also figure 5). The critical values of the field strength given in table I are of course Hartree-Fock values and are expected to shift slightly for fully correlated calculations.

## V. SELECTED QUANTITATIVE ASPECTS

In table II we present the total energies of the seven ground state electronic configurations of the carbon atom. The energy of each state is given at least in the range of field strength within which it represents the ground state (in many cases we have performed calculations for a much wider regime of field strengths). The configurations in table II are labeled by their corresponding numbers introduced in table I. The data of the tables I and II represent the total energy values on a grid of field strengths covering the complete regime  $0 \leq \gamma \leq 10000$  and via interpolation can be used to get the total energies for any field strength.

The most important work in the literature containing results on the spectrum of the carbon atom in

a strong magnetic field is ref. [28]. We have illustrate the data of ref. [28] together with our data (see above) figures 1-4. Unfortunately ref. [28] does not contain a detailed description of the electronic states of the carbon atom considered in their work: the data given for electronic states with  $S_z = -2$  and  $S_z = -3$  cannot uniquely be identified with our electronic configurations since the quantum numbers of the individual one particle functions of their HF procedure have not been specified. Nevertheless we can compare the total energies of the lowest configuration at a fixed field strength. As a general tendency we observe that in most cases our energy values are significantly lower than those of ref. [28]. Indeed, ref. [28] obtained only three different ground state configurations whereas the true picture, as described above, involves seven different electronic configurations and six associated crossovers. One can see in figure 1 that it is difficult to associate the first three  $S_z = -1$  points of ref. [28] presented in this picture with any of our states. On the other hand some energy values given in ref. [28] lie close to our energies which is the case for the configuration  $1s^2 2s 2p_0 2p_{-1}^2$  and we perform the comparison with our results for this state in table III.

A second source of data on the carbon atom in strong magnetic fields is ref. [23]. This work deals exclusively with the high field regime in which the adiabatic approximation represents a reasonable approach to the wave functions and spectrum. The total energies of the ground state of the high field limit are given in ref. [23] for four different values of the field strength in the regime  $42.544 \leq \gamma \leq 2127.2$ . Table IV contains a comparison of those data with our HF data for the high field ground state configuration  $1s 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 6h_{-5}$ . The third and fourth column represent our total energies and those of ref. [23], respectively. As a general tendency our energies are of the order of magnitude of  $0.1keV$  lower than those of ref. [23]. This is a nonnegligible deviation in particular in view of the fact that it exceeds the energy difference to the first excited state shown in column five of table IV and for two points of the lowest field strength the situation is even worse: it exceeds the ionization energy of the atom, i.e. the energy necessary to build the single positive charged ion  $C^+$  (see column six in table IV). We believe that our results are much more accurate than those of ref. [23] since we do not involve any kind of adiabatic approximation and deal with a flexible wave function due to the flexible mesh calculation of our one particle functions.

Figure 6 allows us to add some details to the considerations of the previous section. This figure presents spatial distributions of the total electronic densities for the ground state configurations of the carbon atom. More exactly, this picture allows us to gain insights into the geometry of the distribution of the electron density in space and in particular its dependence on the magnetic quantum number and the total spin. Thereby we can understand the corresponding impact on the total energy of the atom. The first picture in this figure presents the distribution of the electron density in the ground state of the carbon atom at  $\gamma = 0$ . The following pictures show the distributions of the electronic densities at values of the field strength which mark the boundaries of the regimes of field strengths belonging to the different ground state configurations. For the high-field ground state we present the distribution of the electronic density at the crossover field strength  $\gamma = 18.664$  and for three additional values of  $\gamma$  up to  $\gamma = 1000$ .

For each configuration the effect of the increasing field strength consists in compressing the electronic distribution towards the  $z$  axis. However most of the crossovers of ground state configurations involve the opposite effect which is due to the fact that they are associated with an increase of the total magnetic quantum number  $M = \sum_{\mu=1}^6 m_{\mu}$ .

Two issues concerning the results presented above have to be discussed. First, our HF results do not include the effects of correlation. To take into account the latter would require a multiconfigurational approach which goes beyond the scope of the present paper. We, however, do not expect that the



correlation energy changes our main conclusions like, for example, the fact of the crossovers with respect to the different ground states configurations. With increasing field strength the effective one particle picture should be an increasingly better description of the wave function and the percentage of the correlation energy should therefore decrease (see in particular ref. [37]). The concrete values of quantities like, for example, the transition field strengths or the ionization energies, depend however to some extent on the approach used (Hartree-Fock, correlated methods).

Additional consideration are however required for the crossover situation itself which separates different electronic configurations of the ground state and for the other intersections presented in figures 1 to 4. In principle, effects of electronic correlation can turn level crossings into avoided crossings. In this case the classification of the ground state via a single configuration of six one particle states should break down and the discontinuous changes of the slope of the total energies at the points of crossovers should be smoothened out. But we do not expect these effects of correlation to occur for the ground state configurations due to the different symmetries of the configurations involved. Indeed, one can see in table I that all the neighboring ground state configurations have at least either different total magnetic quantum numbers or different total spins. Thus, we do not expect that correlation effects can lead to avoided crossings in the energies of the ground state configurations of the carbon atom.

The second issue relates to effects of the finite nuclear mass. For the case of hydrogen it is well-known that in the high field regime ( $\gamma \gg 10^2$ ) mass correction terms due to the finite nuclear mass become relevant i.e. are no more negligible in comparison with the Coulomb binding energies. The most important mass corrections can be included by replacing the electron mass through its reduced mass and results from the infinite nuclear mass calculations are related to those with the reduced mass via a scaling relation [8,11]. In the case of the much heavier C atom these effects are expected to be suppressed significantly due to the large nuclear mass. In addition the total Coulomb binding energy increases rapidly with increasing nuclear charge number and is therefore for the carbon atom almost two orders of magnitude larger compared to the hydrogen atom. This makes the effects of the finite nuclear mass less important than for hydrogen.

## VI. SUMMARY AND CONCLUSIONS

We have applied our 2D mesh Hartree-Fock method to the magnetized carbon atom. The method is flexible enough to yield precise results for arbitrary field strengths and our calculations for the ground and several excited states are performed for magnetic field strengths ranging from zero up to  $2.3505 \cdot 10^9 \text{T}$  ( $\gamma = 10000$ ). Our considerations focused on the ground state and its crossovers with increasing field strength. It undergoes six transitions involving seven different electronic configurations. For weak fields up to  $\gamma = 0.1862$  the ground state arises from the field-free ground state configuration  $1s^2 2s^2 2p_0 2p_{-1}$  with the total spin  $z$ -projection  $S_z = -1$ . With increasing strength of the field four different electronic configurations with  $S_z = -2$  consequently become the ground state:  $1s^2 2s 2p_0 2p_{-1} 2p_{+1}$ ,  $1s^2 2s 2p_0 2p_{-1} 3d_{-2}$ ,  $1s^2 2p_0 2p_{-1} 3d_{-2} 4f_{-3}$  and finally  $1s^2 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$ . At  $\gamma = 12.216$  we observe the first fully spin polarized configuration  $1s 2p_0 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$  with  $S_z = -3$  to become the ground state of the carbon atom. At  $\gamma = 18.664$  the last crossover of the ground state configurations takes place and ergo for  $\gamma > 18.664$  the ground state wave function is represented by the high-field-limit configuration  $1s 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 6h_{-5}$ ,  $S_z = -3$ .

Our investigation represents the first conclusive study of the ground state of the carbon atom for

arbitrary field strengths. We have obtained a rather intricate sequence of electronic configurations with increasing field strength. This underlines the conjecture that the scenario of ground state crossovers with changing field strength complicates rapidly if we consider neutral atoms with increasing nuclear charge number. Our computations have been performed in the unrestricted Hartree-Fock approximation. For the configurations with  $S_z = -1$  and  $S_z = -2$  (not for those with  $S_z = -3$ ) this means that our one determinantal HF wave functions are not eigenfunctions of the operator of the total spin. An immediate improvement of our approach would therefore require a multiconfigurational study. The development of such a code capable of describing the wave function in arbitrarily strong magnetic fields is however a major task and clearly goes beyond the scope of the present investigation. Putting together what we currently know about ground states of atoms in strong magnetic fields we can conclude that the H, He, Li and C atomic ground states have been identified. This leaves plenty of questions open about the possible ground state configurations of other atoms.

### Acknowledgments

One of the authors (M.V.I.) gratefully acknowledges financial support from the Deutsche Forschungsgemeinschaft. P.S. acknowledges financial travel support by the NSF/DAAD and the hospitality of the Department of Physics of the University of Nevada at Reno.

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## Figure Captions

**Figure 1.** The total energies (in atomic units) of the states of the carbon atom as functions of the magnetic field strength considered for the determination of the ground state electronic configurations

with  $S_z = -1$ . Our results (solid lines) and data taken from ref. [28] (broken lines). Energies and field strengths are given in atomic units.

**Figure 2.** Same as in figure 1 for  $S_z = -2$ , lower field part. Energies and field strengths are given in atomic units.

**Figure 3.** Same as in figure 1 for  $S_z = -2$ , higher field part. Energies and field strengths are given in atomic units.

**Figure 4.** Same as in figure 1 for  $S_z = -3$ . Energies and field strengths are given in atomic units.

**Figure 5.** Energies of the ground state configurations as a function of the field strength. Vertical dotted lines divide regions belonging to different Hartree-Fock ground state configurations. Energies and field strengths are given in atomic units.

**Figure 6.** Contour plots of the total electronic densities for the ground state of the carbon atom. For neighboring lines the densities are different by a factor of  $e$ . The coordinates  $z$ ,  $\rho$  as well as the corresponding field strengths are given in atomic units.

TABLE I. The Hartree-Fock ground state configurations of the carbon atom in external magnetic fields. The configurations, presented in the table are the ground state configurations at  $\gamma_{\min} \leq \gamma \leq \gamma_{\max}$ .

no.	$\gamma_{\min}$	$\gamma_{\max}$	The ground state configuration	$M$	$S_z$	$E(\gamma_{\min})$
1	0	0.1862	$1s^2 2s^2 2p_0 2p_{-1}$	-1	-1	-37.69096
2	0.1862	0.4903	$1s^2 2s 2p_0 2p_{-1} 2p_{+1}$	0	-2	-37.9334
3	0.4903	4.207	$1s^2 2s 2p_0 2p_{-1} 3d_{-2}$	-3	-2	-38.3359
4	4.207	7.920	$1s^2 2p_0 2p_{-1} 3d_{-2} 4f_{-3}$	-6	-2	-41.7369
5	7.920	12.216	$1s^2 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$	-10	-2	-43.6397
6	12.216	18.664	$1s 2p_0 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$	-10	-3	-44.9341
7	18.664	$\infty$	$1s 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 6h_{-5}$	-15	-3	-50.9257

TABLE II. The energies of the ground state configurations of the carbon atom dependent on the magnetic field strength. The figures in paratheses are the numbers of the ground state configurations provided in the first column of table I. Energies and field strengths are given in atomic units.

$\gamma$	$E(1)$	$E(2)$	$E(3)$	$E(4)$	$E(5)$	$E(6)$	$E(7)$
0.000	-37.69096	-37.59928	-37.2188	-36.1170	-35.1186	-24.3112	-22.5588
0.001	-37.6925	-37.6013	-37.2224	-36.122	-35.126	-24.3193	-22.570
0.002	-37.6940	-37.6034	-37.2259	-36.1270	-35.133	-24.3272	-22.580
0.005	-37.6985	-37.6094	-37.2360	-36.1413	-35.152	-24.3496	-22.608
0.01	-37.7059	-37.6193	-37.2526	-36.1641	-35.1827	-24.3853	-22.6539
0.02	-37.7205	-37.6389	-37.2842	-36.2085	-35.2399	-24.4525	-22.7376
0.05	-37.7633	-37.6966	-37.3705	-36.3247	-35.3900	-24.6328	-22.9579
0.1	-37.8302	-37.7882	-37.5010	-36.4932	-35.6027	-24.8959	-23.2743
0.2	-37.9486	-37.9552	-37.7388	-36.7835	-35.9600	-25.3546	-23.8125
0.3	-38.0479	-38.1026	-37.9579	-37.0387	-36.2653	-25.7617	-24.2813
0.4	-38.1302	-38.2323	-38.1624	-37.2716	-36.5376	-26.1358	-24.7067
0.5	-38.1973	-38.3464	-38.3541	-37.4881	-36.7864	-26.4865	-25.1007
0.6	-38.2510	-38.4467	-38.5339	-37.6912	-37.0170	-26.8187	-25.4706
0.7	-38.2927	-38.5346	-38.7033	-37.8830	-37.2329	-27.1362	-25.8211
0.8	-38.3238	-38.6116	-38.8632	-38.0650	-37.4364	-27.4411	-26.1554
0.9	-38.3453	-38.6788	-39.0145	-38.2385	-37.6293	-27.7351	-26.4758
1.	-38.3582	-38.7373	-39.1577	-38.4043	-37.8130	-28.0195	-26.7843
1.5	-38.3192	-38.9225	-39.7776	-39.1406	-38.6242	-29.3275	-28.1888
2.	-38.1549	-38.9770	-40.2769	-39.7621	-39.3061	-30.4938	-29.4282
3.	-37.6035	-38.8418	-41.0477	-40.7780	-40.4222	-32.5445	-31.5925
4.	-36.8901	-38.5088	-41.6319	-41.5886	-41.3180	-34.3404	-33.4807
5.	-36.0969	-38.0551	-42.1016	-42.2549	-42.0608	-35.9601	-35.1815
7.		-36.9093	-42.8151	-43.2771	-43.2195	-38.8325	-38.1971
8.		-36.2426	-43.0841	-43.6685	-43.6734	-40.1320	-39.5620
10.		-34.7539	-43.4769	-44.2659	-44.3872	-42.5277	-42.0799
12.			-43.7032	-44.6615	-44.8905	-44.7094	-44.3749
15.			-43.7842	-44.9571	-45.3348	-47.6770	-47.5002
20.			-43.3767	-44.8468	-45.4465	-52.0282	-52.0890
30.			-41.1418	-43.0912	-44.0660	-59.2747	-59.7433
40.			-37.6519	-39.9996	-41.2855	-65.2949	-66.1073
50.			-33.3211	-36.0197	-37.5718	-70.5187	-71.6285
100.				-8.865	-11.3693	-90.2751	-92.4552
200.				+60.973	+57.3384	-116.4070	-119.8127
500.				+307.31	+301.1777	-163.209	-168.5248
1000.				+754.1	+746.589	-209.98	-217.1413
2000.						-268.711	-278.1612
5000.						-368.1	-381.8097
10000.						-463.7	-480.875

TABLE III. The energy of the state  $1s^2 2s 2p_0 2p_{-1}^2$  of the carbon atom in magnetic fields compared with results by Jones et al(1996). Energies and field strengths are given in atomic units.

$\gamma$	$E(1s^2 2s 2p_0 2p_{-1}^2)$	$E$ [28] $S_z = -1$
0.216	-37.7779	-37.793
0.504	-38.1345	-38.134
0.720	-38.3254	-38.325
2.16	-38.7188	-38.713
3.6	-38.4076	-38.376
5.04	-37.7940	-37.677
7.2	-36.5467	-36.239
8.64	-35.5527	-35.196
14.4	-30.6343	-29.969
21.6	-23.0362	-21.472

TABLE IV. The energies of the high-field ground state of the carbon atom  $E(C)$ , its first high-field excited state ( $1s 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 7i_{-6}$ ) and the energy of the ion  $C^+$  compared with the adiabatic results by Neuhauser et al (1987) for the high-field ground state.

$B$ ( $10^{12}$ G)	$\gamma$	$E(C)$ (keV)	$E(C)$ [23] (keV)	$E(1s 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 7i_{-6})$ (keV)	$E(C^+)$ (keV)
0.1	42.544	-1.83895	-1.678	-1.82464	-1.78348
0.5	212.72	-3.33639	-3.22	-3.30957	-3.22647
1.0	425.44	-4.31991	-4.20	-4.28530	-4.17396
5.0	2127.2	-7.73528	-7.60	-7.67499	-7.46051

Figure 1.

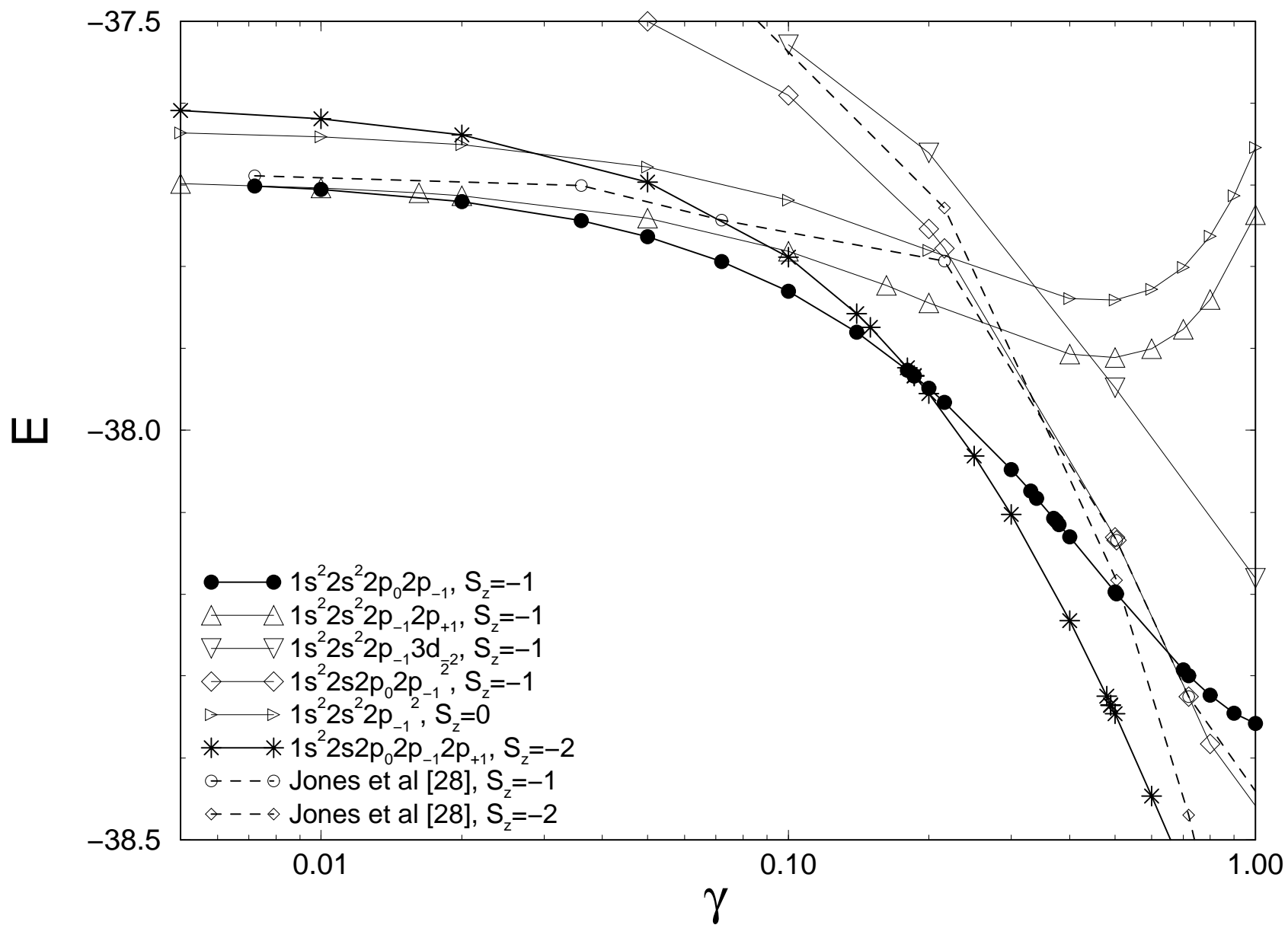




Figure 2.

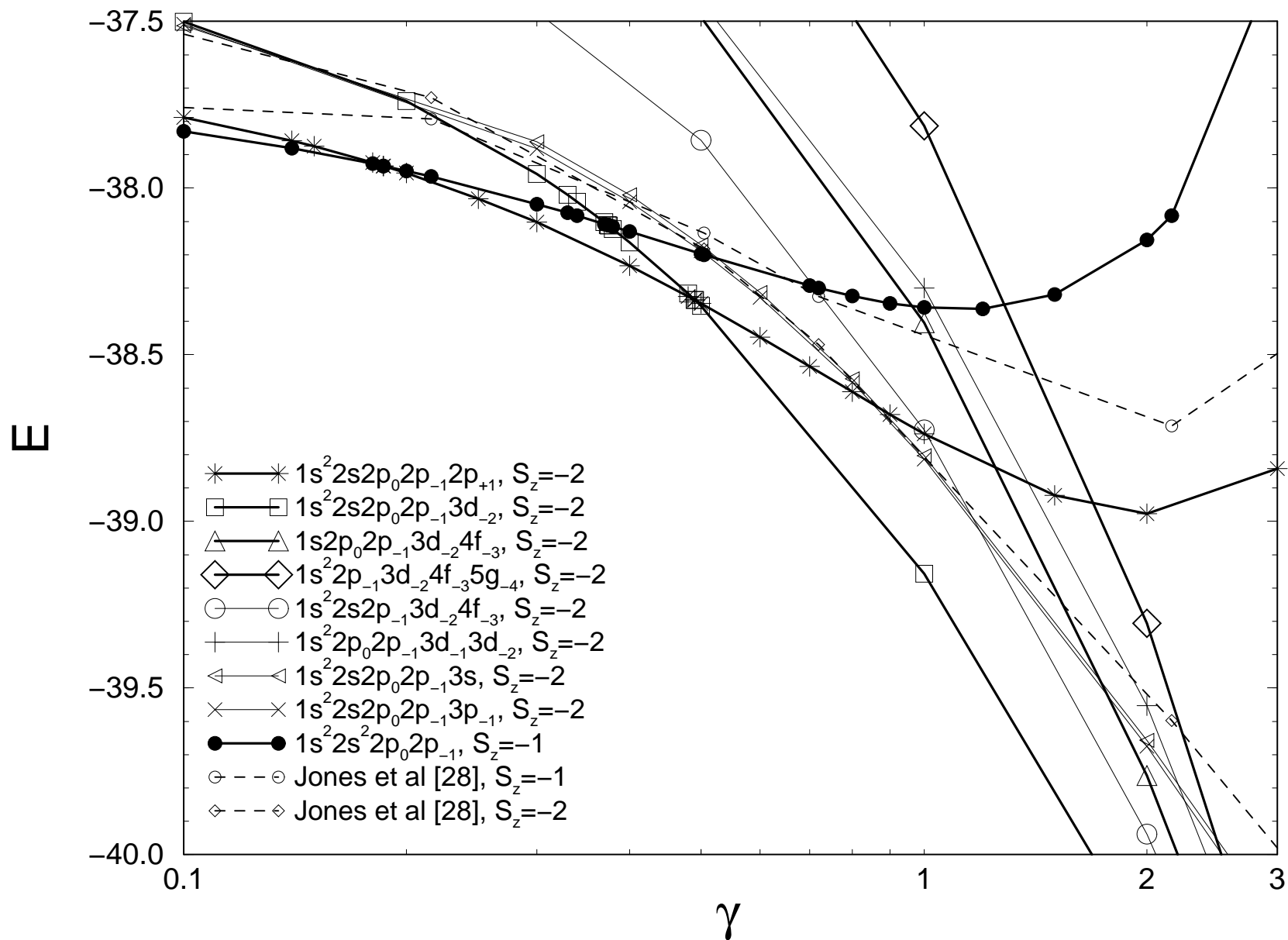


Figure 3.

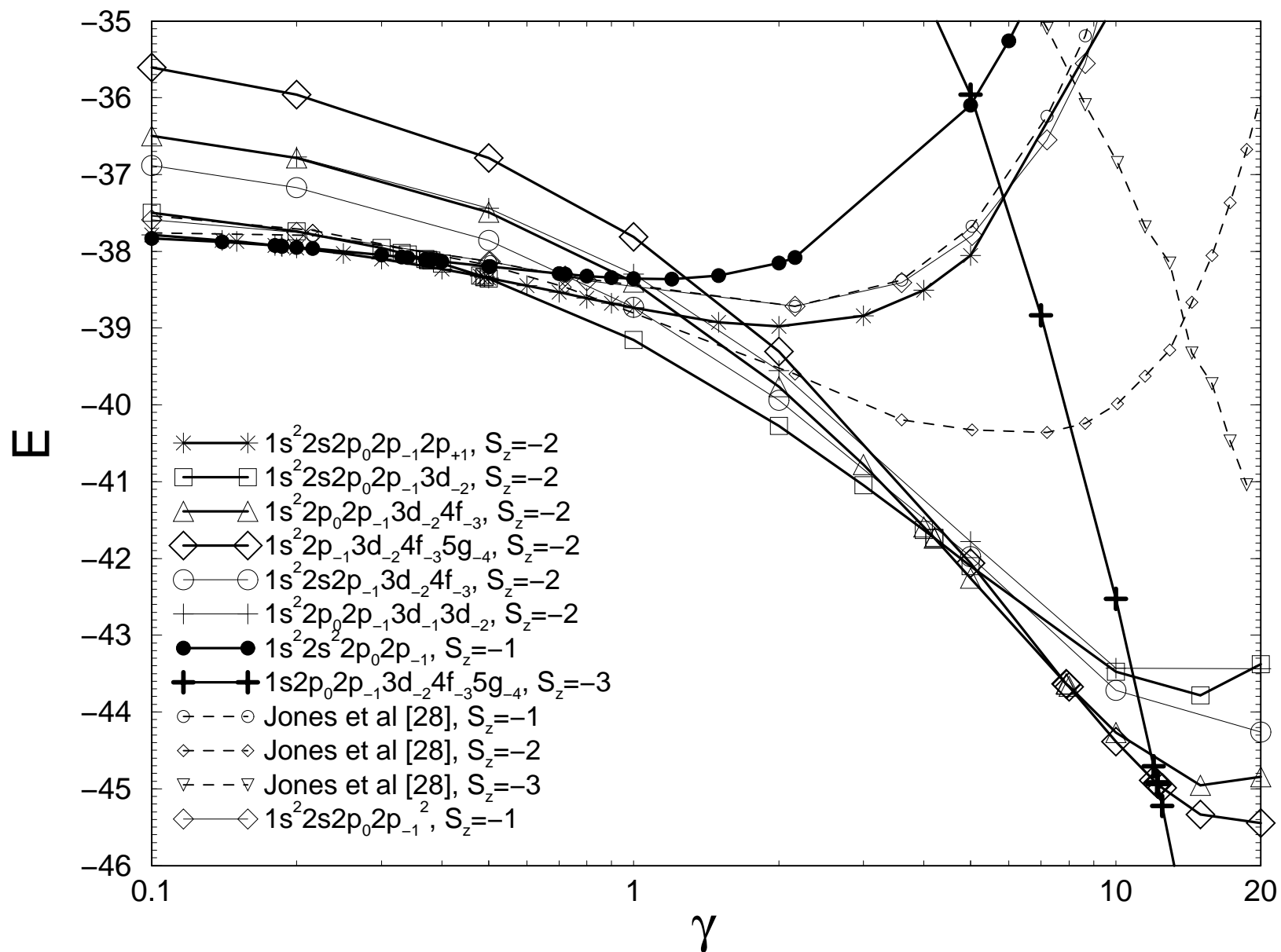
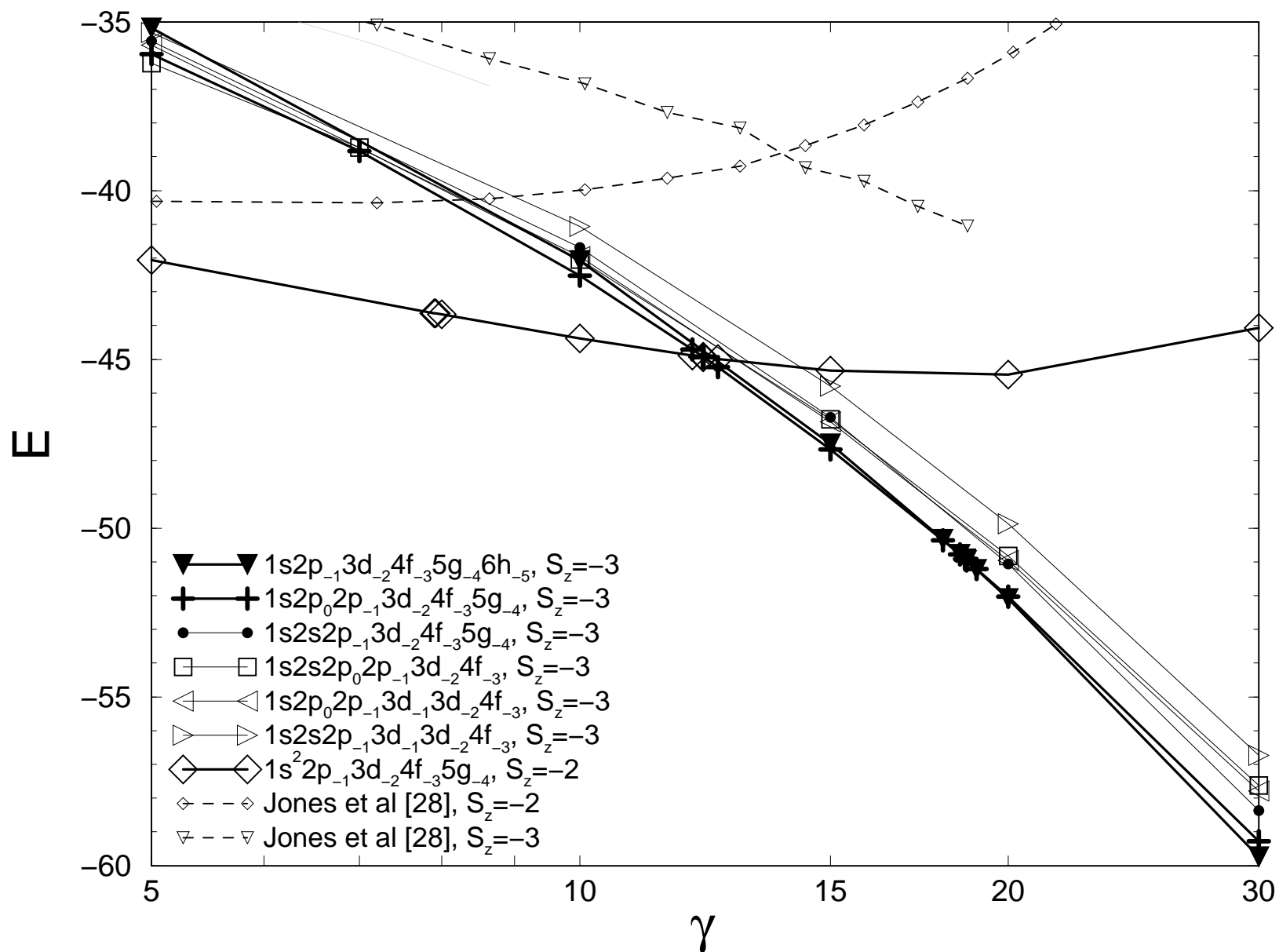


Figure 4.



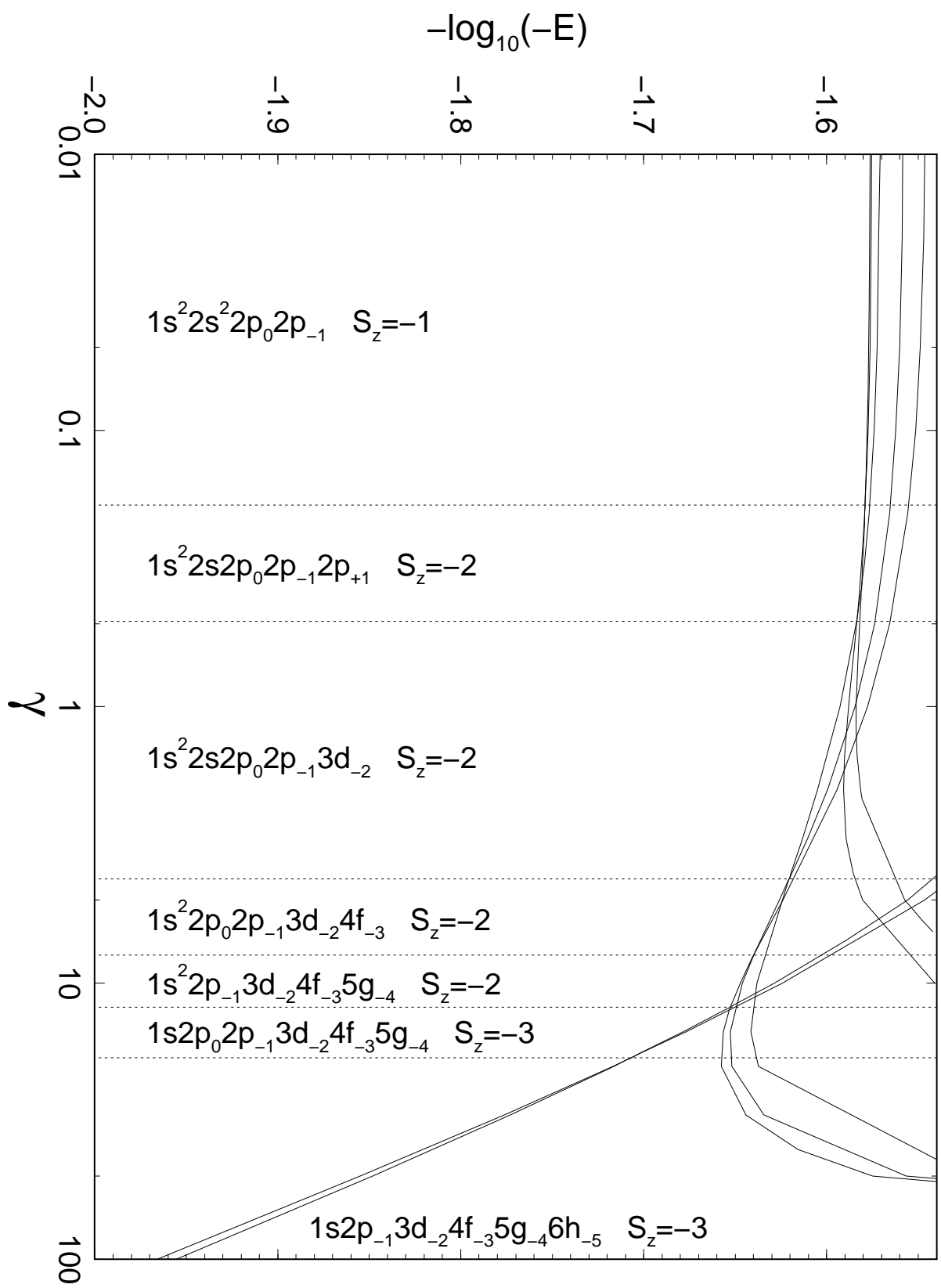


Figure 5.

